ACCURACY OF WWR–M CRITICALITY CALCULATIONS WITH CODE MCU–RFFI*

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ABSTRACT

The scattering and deviation of fuel element parameters by manufacturing, approximations of the reactor structure in the computer model, the partly inadequate neutron cross sections in the computer codes etc. lead to a discrepancy between the reactivity computations and data. We have compared reactivity calculations using the MCU–RFFI Monte Carlo code of critical assemblies containing WWR–M2 (36 enriched) and WWR–M5 (90%) fuel elements with benchmark experiments. The agreement was about $\Delta\rho \simeq \pm 0.3\%$. A strong influence of the water ratio on reactivity was shown and a significant heterogeneous effect was found. We have also investigated, by full scale reactor calculations for the RETR program, the contribution to the reactivity of the main reactor structure elements: beryllium reflector, experimental channels, irradiation devices inside the core, etc. Calculations show the importance of a more thorough study of the contributions of products of the (n, α) reaction in the Be reflector to the reactivity. Ways of improving the accuracy of the calculations are discussed.

INTRODUCTION

1.1 WWR–M description. **The reactor WWR–M went critical in 1959. Its core contains 271 hexagonal cells with cross section of $10.61\ cm^2$ each containing fuel assemblies (FA) with the height of fuel $50\ cm$, control and safety rods, replaceable beryllium assemblies and experimental devices[1]. The cylindrical beryllium reflector (height $59\ cm$, diameter $93.6\ cm$ and average thickness $16.5\ cm$) contains 9 horizontal and 13 vertical channels. In comparison with the Budapest reactor (397 cells for FA with the same cross section area, but with the height of fuel $60\ cm$ instead of $50\ cm$[2] the reactor at Gatchina has a 1.8 time smaller volume of the core and therefore is more difficult to convert to LEU fuel.**

The reactor fuel assemblies WWR–M5 have the world's highest specific heat–transfer surface per volume of the core: $\xi = 6.6\ cm^2/cm^3$[3]. This allows one to remove the maximum specific power $(0.9 \pm 0.1\ MW/l)$ in a pool reactor. Reactor is operated at the nominal power of 18 MW. The high density of ^{235}U in WWR-M5 fuel elements ($66\ g^{235}$U/FA, 90% of enrichment) allows one to put experimental devices of significant size inside the core and to carry out unique fundamental investigations with cold, ultra cold and polarized neutrons[4].

In order to study the feasibility of the enrichment reduction in the WWR - M reactor a typical configuration of the core with a source of cold neutrons (UCNS) is chosen (Fig.1). The core loading includes 144 WWR–M5 FA with (UO_2+Al) fuel elements (FE). The FE thickness is equal to $1.25\ mm$ and the thickness of the meat is $0.39\ mm$ (Fig.2). The distribution of the fuel in the FA is presented in Tab.1.

Table 1: **WWR–M FA specification** ($H_{FA} = 50\ cm$, $S_C = 10,609\ cm^2$, $V_{FA} = 530,44\ cm^3$, **lattice spacing** $a = 3,5\ cm$).

	Fuel assembly type	WWR–M2 UAl alloy	WWR–M5 UAl alloy	WWR–M5 UO_2+Al
1	^{235}U enrichment, W %	36	90	90
	^{238}U, W %	63.6	9.0	9.0
	^{234}U, W %	0.4	1.0	1.0
2	U Meat density, g/cm^3	1.352	0.7832	1.087
	^{235}U Meat density, g/cm^3	0.4868	0.7048	0.9785
3	FE wall/clad/meat thickness, mm	2.5/0.9/0.7	1.25/0.36/0.53	1,25/43/0,39
	FE dimension hex/cyl$\cdots$/rod, cm	3.2/2.2/1.1	3.35/2.79/2.23/1.67/1.11/0.55	
4	Meat ratio in cell, $\omega_M = S_M/S_C$	0.12547	0.17278	0.12716
	Measured H_2O ratio, $\omega_{H_2O}^{EXP}$	0.542(34)	0.571(4)	—
	Calculated H_2O ratio, $\omega_{H_2O}^{TH}$	0.5671	0.5708	0.5758
5	^{235}U mass, g^{235}U/FA	32.4	64.6	66.0
	^{238}U mass, g^{235}U/FA	57.2	6.5	6.6

A source of cold and ultra cold neutrons (UCNS) is situated in the middle of the core. It occupies 69 cells. The volume of the zirconium chamber with liquid hydrogen is about $1\ l$. It is cooled by helium. For irradiation of materials (various kinds of steel) ampoules of one cell size are used. The loading of 14 ampoules corresponds to the usual volume of tests. The ampoules are placed near the minimum shield thickness of UCNS. The device for irradiation of materials by fast neutrons occupies 7 cells. In order to reduce the induced activity it has a cadmium screen. Fourteen beryllium blocks are situated in front of horizontal channels to reduce the flux of fast neutrons at the channel bottoms and thus for increasing of their resource. For reduction of gamma radiation, 4 blocks of lead are placed opposite to the horizontal channel II. Opposite to the graphite thermal column on line *"A"* a row of 10 lead blocks is placed to reduce its gamma heating.

The beryllium reflector is cooled by water, flowing in vertical channels. The water ratio in beryllium is 2.5%. In the reflector 9 horizontal channels and 13 vertical ones are available. The horizontal channels II, IV, VII and IX reach the core, and the horizontal channels I, III, V, VI and VIII penetrate into the reflector by $10\ cm$. Holes for the vertical channels B1,2,3,11,12 and 13 thread the whole reflector, and B4,5,6,7,8,9 and 10 reach only the horizontal channels. Channel B7 is empty, the other vertical channels are filled with water.

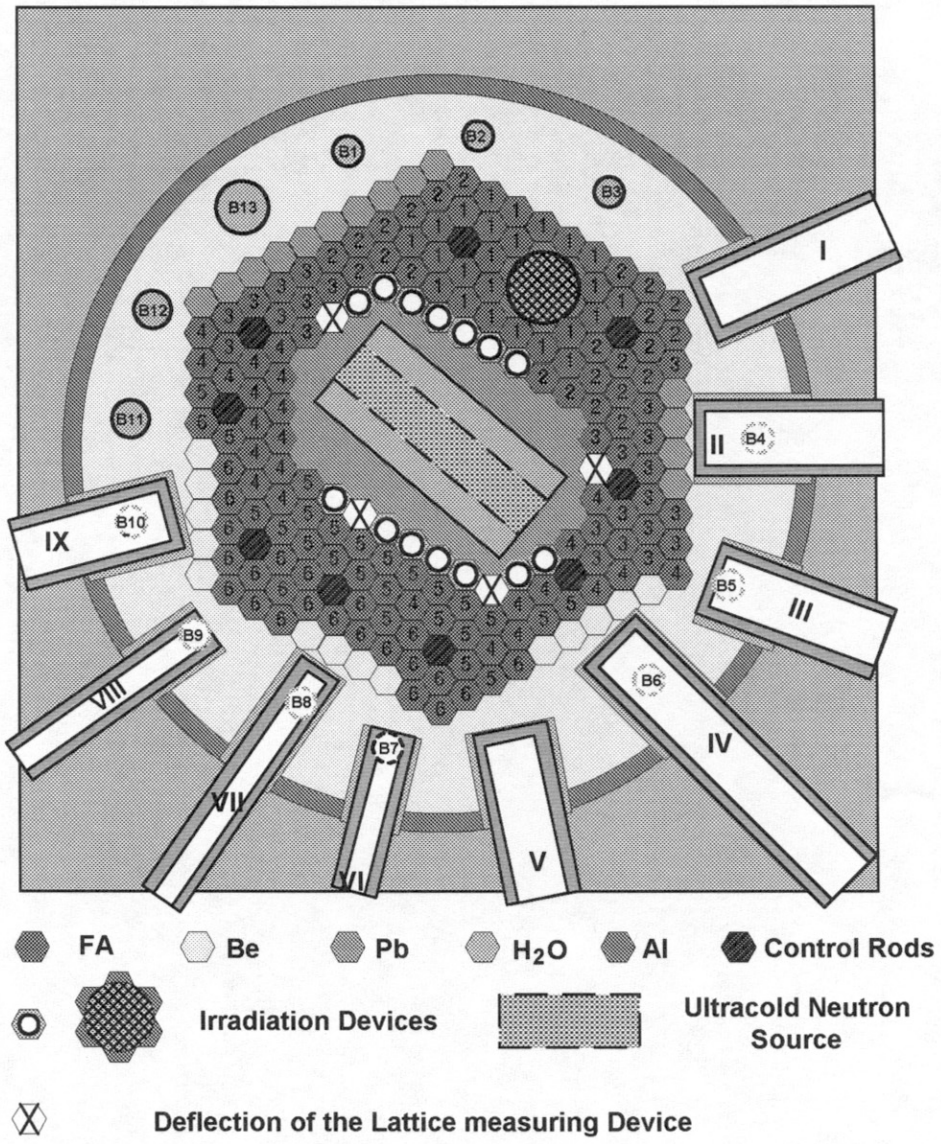


Fig.1.WWR-M core for LEU-HEU conversion study. 1-6 are steps of burnup for EOEC

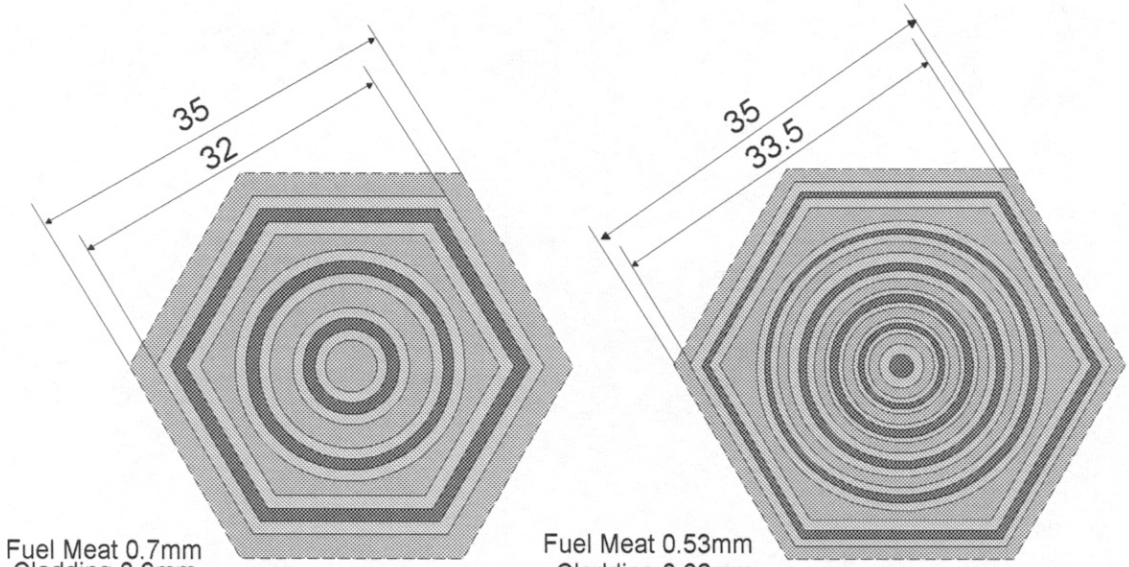
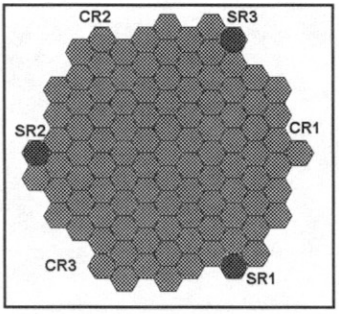
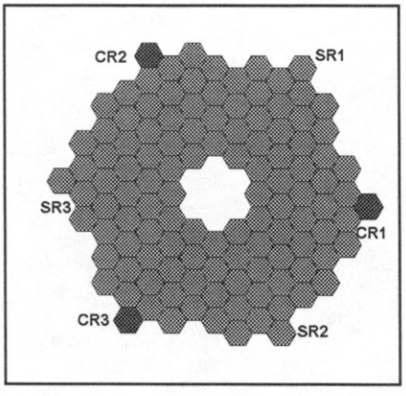


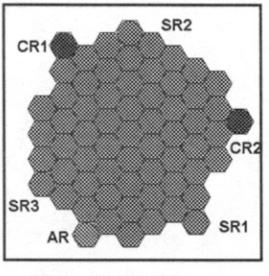
Fig.2. WWR - M2 and WWR - M5 Fuel Assembly



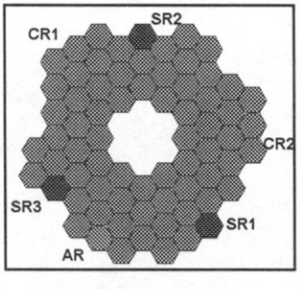
96 WWR-M2 FA



111 WWR-M2 FA

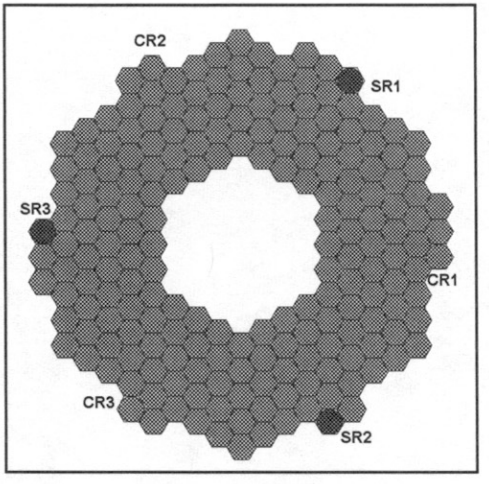


57 WWR- M5 FA

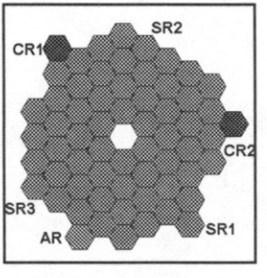


64 WWR- M5 FA

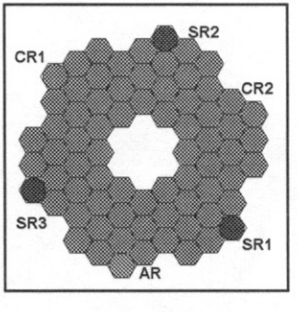
Fig.3.Configurations of critical assemblies for benchmark



189 WWR-M2 FA



56 WWR-M5 FA



66 WWR -M5 FA

The control system of the reactor consists of 9 control rods containing B_4C.

The places at which the neutron flux will be compared after enrichment reduction are the $1\ l$ volume of UCNS, the total volume of ampoules, the 7 cell water trap for irradiation, typical vertical channels B2, B8, B13 and the bottoms of typical horizontal channels II, IV, VIII.

1.2 Critical assemblies description. Configurations of critical assemblies are presented in Fig.3. The assemblies WWR–M2 were mounted on a plate made from an aluminum alloy $40\ mm$ thick. The plate has holes ($\o 14\ mm$) for FA legs. The control and safety rods (CR and SR) were made from B_4C, coated with the aluminum alloy. The walls of CR and SR channels are made of aluminum alloy only. There is water inside the CR channels, and air inside the SR channels. The SR were withdrawn. In the critical assemblies WWR–M2 the FA with 32.4 g ^{235}U/FA (36%) were used.

In the assemblies with WWR–M5 FA the SR channels were filled also with water. The absorber of the automatic control rod (AR) is steel ($\o 25\ mm$). In an assembly WWR–M5 the FA which have $64.6\ g^{235}$U/FA (90% enrichment) were used. Due to the fact that the reactivity strongly depends on the water ratio in the core (ω_{H_2O}), it was measured experimentally. The values of $\omega_{H_2O}^{EXP}$ (with a double error, i.e. at 90% CL) are shown in Tab.1. The experimental error of the critical mass was determined above all on small "dislocations"[1] of the FA which changes the average amount of water in a core, and the dispersion of the FA parameters by the manufacturing. The latter error was determined by completely changing all FA in an assembly. The results of measurements and experimental errors are presented in report[5]. The accuracy of critical mass evaluation is $0.2 - 0.3\%$ for the WWR–M2 and $0.7 - 0.8\%$ for the WWR–M5. It can lead to an experimental error in the determination of the criticality up to $\sigma^{EXP} = \Delta K^{EXP}/K^2 = 0.2\%$.

1.3 Code MCU–RFFI For most computations of this report the code MCU – RFFI was used. The MCU–RFFI is a generalized-geometry Monte Carlo code for reactor criticality calculations and neutron transport simulation in fission reactors. This code was developed in the Russian Federal Center "Kurchatov Institute"[6–8].

The evaluated neutron cross section library DLC/MCUDAT was used for neutron transport simulation. For the energy dependence of the neutron cross sections several libraries were used in the epithermal region (for energies above $1.0\ eV$) and in the thermal energy region (below $1.0\ eV$). The resolved resonance cross sections of uranium were calculated using Breit-Wigner or Adler-Adler formulas with resonance parameters taken from the library LIPAR[7] for each energy point. Doppler broadening was taken into account. The unresolved resonance cross sections were calculated using a sub-group approximation. In total, 23 groups above $1.0\ eV$ were used. The cross section library TEPKON[7] was used to simulate the process of neutron thermalization (40 groups transport approximation). Angular distributions of scattered neutrons were simulated using the model of an ideal

[1] The FA which are inserted into sockets of a lattice can diverge in the upper part ("dislocate themselves") and increase the light water gap between them.

single atom gas or the model of an ideal heavy atom gas. The TEPCON library of neutron cross sections for the hydrogen of a water molecule were calculated in the noncocherent Gauss approximation with the use of an experimental phonon spectrum[7]. The program has a universal geometrical module for the description of complex 3D geometry.

BENCHMARK CALCULATIONS

2.1 Heterogeneous effect. In the heterogeneous calculations the computer model reproduced the structure of FA completely: the H_2O gap, geometry of FE, meat and cladding. In the homogeneous model all these elements are mixed inside a cell in the appropriate proportions. By the definition the heterogeneous effect is a difference between the reactivity calculations in both models. The comparison of the heterogeneous and homogeneous calculations with the code MCU–RFFI is presented in Tab.2. The calculation for the hexagonal cell of infinite length in an infinite lattice (this geometry was taken into account with transversal boundary conditions) shows, that the heterogeneous effect for the WWR-M5 FA is small and negative. This means that the self–shielding of ^{235}U in the thermal region is not compensated by a reduction of the resonant capture by the small quantity of ^{238}U. The heterogeneous effect for an infinite lattice with axial water reflector is larger.

In an assembly of finite size the difference is much higher (Tab.2). Due to a large free path of neutrons in the aluminum cladding ($\lambda_{Al} \simeq 12\ cm$) and in the meat the leakage of neutrons in the heterogeneous FA is higher than in the homogeneous one. Due to the significant heterogeneous "gun effect" the homogeneous approach is not correct ($\rho_5^{het} - \rho_5^{hom} = -2.13(7)\%$).

2.2 Benchmark calculations. The size of the water trap, the number of the FA in the critical assembly are presented in Fig.3. The tails of FA were taken into account (length $3\ cm$, 42%Al). The effect due to the water displacement by tails reduces the reactivity of the assemblies by less than 0.3%.

Direct measurements show that the reactor PIK fuel (90% enriched) contains about 1% of ^{234}U, i.e. $^{234}\mathrm{U}/^{235}\mathrm{U} = 1,1 \cdot 10^{-2}$[9]. In the certificates accompanying the WWR-M2 and WWR-M5 FA the concentration of ^{234}U is not specified. Therefore in all calculations it was assumed to be equal to $^{234}\mathrm{U}/^{235}\mathrm{U} = 1.1 \cdot 10^{-2}$. As already mentioned, the reactivity of assemblies strongly depends on the content of water in FA, ω_{H_2O}. For the assembly of WWR-M2 without trap, according to the calculations with the code MCU, the derivative is equal to $\omega_{H_2O}\partial\rho_2^{het}/\partial\omega_{H_2O} = 0.35(4)$. Unfortunately, the experimental accuracy of determination of $\omega_{H_2O}^{EXP}$ for the WWR-M2 is rather poor (Tab.1). That can lead to a large error in the value of the reactivity: $\pm 2\%$. To diminish the uncertainty a value of $\omega_{H_2O}^{TH}$ was chosen (inside the limits of errors $\Delta\omega_{H_2O}^{EXP}$) such as to ensure the value of K^{het} to be close to 1 for an assembly without a trap. This value of $\omega_{H_2O}^{TH} = 0.5671$ was used for both assemblies with a trap (for the assembly with $N_{WT} = 37\ cells$ and for the assembly $N_{WT} = 7\ cells$). As one can see from Tab.3 the average of three assemblies $\bar{\rho}_2^{het} = [-0.06(0.26)]\%$ is close to zero. (In brackets the scattering of the results is shown.) The square root of the variance, significantly exceeds the statistical error of the calculation. This

is due to experimental errors, to manufacturing deviations and to the insufficient accuracy of the computer model.

The WWR–M5 FA contain a little bit less ^{235}U than standard FA ($64.6\ g^{235}\mathrm{U}/FA$ instead of $66\ g^{235}\mathrm{U}/FA$ Tab.1). The water ratio in FA ($\Delta\omega^{EXP}/\omega^{EXP} = 0.35\%$) is determined much more precisely. This allows us to use the value of ω^{EXP} in the calculations without any preliminary fit. For four values of N the mean reactivity is equal: $\bar{\rho}_5^{het} = [+0.17(0.30)]\%$. In this case, without any fit, the computations describe the experimental data with sufficient accuracy.

Table 2: **Heterogeneous effect for WWR–M5 FA (64,6 g^{235}U/FA, ω_{H_2O} =0,5708).**

		ρ^{het}, % $[K^{het}]$	ρ^{hom}, % $[K^{hom}]$	$\rho^{het} - \rho^{hom}$ %
1	Infinite core	44.82(1) [1.8121(2)]	44.96(0) [1.8167(1)]	−0.14(1)
2	Infinite core with axial reflector (metal–water FA tail $3cm$ and further thick water layer)	38.62(3) [1.6293(7)]	39.02(2) [1.6399(5)]	−0.40(3)
3	Critical assembly with 57 FA	−0.10(5) [0.9990(5)]	2.03(5) [1.0207(5)]	−2.13(7)

In table 3 the results of testing the code MCU–RFFI for benchmarks PIK with low H/^{235}U ratio[10–11] and for VVR–440 type lattice with high H/^{235}U ratio (and low enrichment)[12] are shown for comparison. The mean value is close to zero and the scattering is rather low: about 0.3%. Thus, we can recommend the code MCU–RFFI for HEU–LEU neutronic computations.

Table 3: **Benchmark computations with code MCU–RFFI.**

	Critical assemblies	Number of Cr.Ass.	Enr., %	H/^{235}U	$\overline{\rho}^{het}$, %
1	WWR–M2	3	90	242	−0.06(26)
2	WWR–M5	4	90	122	+0.17(30)
3	PIK–04 [10]	7	89.9	27.0	−0.02(8) ±0.13[1)]
4	PIK–01 [11]	8	89.9	25.8	+0.03(7) ±0.19[1)]
5	ZR–6 (VVR–440) [12]	13	3.6	827	−0.06(21)

[1)] With ± the possible difference due to experimental uncertainty is shown.

REACTIVITY OF FRESH WWR–M CORE

For a reliable calculation of the full scale WWR–M reactor it is important to know the contribution of the main reactor structure elements to reactivity (Tab.4).

Table 4: **Contribution of the WWR–M structure elements to reactivity.**

		ρ^{het}, %	$\Delta\rho$, %
1	Infinite core with infinite FA	44.81(1)	$[k_\infty^{het}$ =1.8141(2)]
2	Axial H_2O reflector	38.64(2)	$\rho_2 - \rho_1$ =–6.17(2)
3	144 FA with H_2O reflector	–2.68(8)	$[\Delta\rho_{het}$ =–1.94(11)]
4	Core with Be reflector	14.83(6)	$[\Delta\rho_{het}$ =–1.02(8)] $\rho_4 - \rho_3$ =17.51(10)
5	Reflector with hor. and vert. channels	11.96(6)	$\rho_5 - \rho_4$ =–2.87(9)
6	14 Be → 14 Pb blocks change	11.45(6)	$\rho_6 - \rho_5$ =–0.51(9)
7	CNS + 14 ampoules	13.93(6)	$\rho_7 - \rho_6$ = +2.48(9)
8	Cd in 7 cells water trap	12.91(6)	$\rho_8 - \rho_7$ =–1.02(9)

Fuel assemblies WWR–M5 with (UO_2+Al) dispersion fuel used in the reactor contain more water and more uranium than the ones used in the experiment (Tab.1). The K_∞ for this FA is higher. Never the less the core configuration with 144 FA (Fig.1) in pure water has a negative reactivity. The heterogeneous effect is still evident: $\Delta\rho_{het} = -1.9(1)\%$.

The beryllium reflector without channels gives a high positive contribution to the reactivity: $17.5(1)\%$. The heterogeneous effect is going down ($\Delta\rho_{het} = -1.0(1)\%$) owing to a better return of neutrons from the reflector. Due to the high contribution of the reflector it must be modelled very accuratly. So, the layer of water (85 on thick) behind the Be reflector contributes $\Delta\rho = +1.3(1)\%$ in reactivity. The contribution of the horizontal and vertical channels amounts to $\Delta\rho_C = -2.9(1)\%$. Change of 14 outer Be blocks for 14 Pb ones (Fig.1) is equivalent to $\Delta\rho_{Pb} = -0.5(1)\%$ in reactivity. Computer model of the Be reflector is preliminary and it should be refined in future.

Experimental facilities in the middle of the core (UCNS with Pb shielding, 14 ampoules etc) being inserted instead of water give a positive reactivity contribution: $\Delta\rho_{EF} = +2.5(1)\%$. The Cd–shielding in the 7 cells water trap has a negative reactivity: $\Delta\rho_{Cd} = -1.0(1)\%$. Now the content of ampoules and the water content in UCNS–shielding are known very approximately. These values will be defined more exactly in future. The best way to verify the computer model of Be reflector and experimental devices is to compare the computations with experiment. The data are now under preparation.

FUEL BURNUP

4.1 Reactor burnup model in the MCU–RFFI code was an equilibrium cycle in which 24 fresh FA were loaded at the beginning of each cycle and discharged after remaining in the core for 6 cycles. The fuel management strategy used in this analysis was to load the lowest burnup fuel into the region of the core with the lowest flux and gradually move the fuel into the highest flux. This in/out strategy[13] provides a flatter energy release distribution. The reactor is running for 21 full power days (fpd) at a power level of 18MW and then is shut down for 14 days. The fuel discharge burnup at the end of equilibrium cycle (EOEC) is 29%. At the beginning of the equilibrium fuel cycle (BOEC) the mean fuel burnup in the core is about 10%. Till 1999 reactor WWR–M has produced 197MWy of energy.

Equilibrium core burnup results. The BOEC burnup leads to the loss of reactivity $\Delta\rho_{BOEC} = -3.6(1)\%$ (Tab.5). This value includes the absorption of one effective fission product. The equilibrium (^{135}Xe+^{105}Rh) absorption is equal to $\Delta\rho_{Xe} = -3.9(1)\%$.

Table 5: **Fuel burnup results.**

		ρ^{het}, %	$\Delta\rho$, %
1	**Fresh fuel**	**12.91(6)**	$\Delta\rho_{het}$ **=–1.13(8)**
BOEC			
2	**Fuel burnup**	**9.33(6)**	$\rho_2 - \rho_1$ **=–3.58(9)**
3	**Sm poisoning**	**7.83(6)**	$\rho_3 - \rho_2$ **=–1.50(9)**
4	**Xe, ^{105}Rh poisoning**	**3.97(7)**	$\rho_4 - \rho_3$ **=–3.86(9)**
EOEC			
5	**Fuel burnup**	**7.63(6)**	$\rho_5 - \rho_1$ **=–5.28(9)**
6	**(Xe+Sm) poisoning**	**3.01(6)**	$\rho_6 - \rho_5$ **=–4.62(9)**
7	**^{6}Li poisoning**	**2.36(7)**	$\rho_7 - \rho_6$ **=–0.65(9)**

EOEC burnup amounts to a loss of reactivity of $\Delta\rho_{EOEC} = -5.3(1)\%$. The Xe, Sm, Rh poisoning adds the value $\Delta\rho_{pois} = -4.6(1)\%$. At the EOEC we have a rather high reactivity excess: $\Delta\rho = 3.0(1)$. But the Be poisoning by the Li and ^{3}He must be taken into account[14].

4.2 Beryllium poisoning effect appears due to ^{9}Be$(n,\alpha)^6$Li reaction in which the ^{6}Li with high thermal neutron absorption cross section is produced. If lithium absorption is in equilibrium with production the contribution of ^{6}Li poisoning in reactivity is equal to $\Delta\rho_{Li} = -0.65(9)\%$. Tritium is generated by the reaction ^{6}Li(n,α)T. Tritium decays into ^{3}He and after the reaction ^{3}He(n,p)T the amount of T increases linearly with full released energy $< Pt >$ (if the tritium leakage out of a reflector is zero). For equilibrium fuel cycle ($21fpd + 14$ days shut down) at 18MW the absorption in ^{3}He doubles the loss of reactivity due to ^{6}Li, and the final reactivity excess is $\rho^{het} = +1.7(1)\%$. If before the start the reactor was shut down for a couple

of month, the loss of reactivity due to ^{3}He could be several times higher. But it is hard to believe that during 40 years tritium did not partly leak out. Experimental data about tritium content in beryllium would help.

CONCLUSIONS

The benchmark calculations of reactivity of WWR–M2 and WWR–M5 critical assemblies demonstrate the scattering of code MCU–RFFI results by about 0.3%. For such an accuracy one needs to know reliably the water ratio in the core. Also the heterogeneous effect must be taken into account very carefully. For full scale reactor calculations the beryllium reflector due to the large contribution to reactivity must be reproduced in the computer model with all peculiarities (experimental channels, water behind beryllium etc). The structure and materials of experimental facilities inside the core must be known in all possible details. For the definition of Be reflector poisoning it is necessary to determine the value of lithium and especially of tritium leakage. The diffusion coefficients with temperature dependence must be measured for leakage calculations. Direct measurements of Li and T content are also desirable. As a matter of fact the programme of comparing the full scale reactor calculations with data for WWR–M core must be carried out. Only after that the absolute accuracy $0.5-1\%$ in reactivity needed for RERTR programme could be achieved.

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